Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Density Functional Study of the magnetic structure on spin frustrated $MnSb_2S_4$ and Sr_2MOsO_6 (M = Cu, Ni) CHUAN TIAN, CHANGHOON LEE, ERJUN KAN, North Carolina State University, FANG WU[1], Nanjing Forestry University, MIKE WHANGBO, North Carolina State University — We explored the electronic structures of two spin-frustrated magnetic systems monoclinic $MnSb_2S_4$ and Sr_2MOsO_6 (M = Cu, Ni) on the basis of first principles DFT calculations. The spin exchanges of $MnSb_2S_4$ are frustrated within each MnS_4 chain and between adjacent MnS_4 chains, which explains the observed helical spin order of $MnSb_2S_4$. We predict that $MnSb_2S_4$ is multiferroic with ferroelectric polarization of $\sim$14 $\mu C/m^2$ along the chain direction, and a field-induced reversal of the ferroelectric polarization occurs by reversing the direction of the helical spin rotation. The ordered double perovskites Sr_2MOsO_6 (M = Cu, Ni), reported to be half-metallic, are found to be magnetic insulators. The magnetic structures of Sr_2MOsO_6 were probed by evaluating their spin exchanges.

[1]People's Republic of China

Chuan Tian
North Carolina State University

Date submitted: 11 Nov 2010 Electronic form version 1.4